NSC226971

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 162 °C

Global applicability domain: Inside

Local applicability domain index: 4.67e-01

Confidence level: 6.49e-01

Nearest Neighbors from the Training Set

Image not found
Isopropyl beta-D-1-
thiogalactopyranoside
Measured: 121
Predicted: 132